Modeling open-flow steam reforming of methanol over Cu/ZnO/Al2O3 catalyst in an axisymmetric reactor for hydrogen production

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Résumé en anglais	This paper describes a CFD study of the steam-reforming process (SRP) of methanol in a short pseudo-contact time reactor of fixed bed type, in axi-symmetric conditions. The SRP is important sake for hydrogen production, and the design /scale-up/control of the industrial processes in the future are supported by a reliable knowledge and prediction of the catalytic reaction. The difficulty of determining the reaction scheme and the associated constants is well-known, due to the necessity of identifying the reaction kinetics in purely chemical regime, meaning with a perfect homogeneity and flow independence. Practically these ideal conditions, albeit assumed, are not fulfilled so that the intrinsic chemical kinetics is not reached. For the case of SRP, we have attempted here to validate the Peppley's model by a numerical modelling reproducing exactly the local conditions in the experimental duct, accounting for gradients in the cross section. The numerical results show the same trends than the experimental one, but with a slight shift of 20% as a consequence of the reactor heterogeneity. This result seems acceptable to validate the use of the Peepley's model for further studies in other types of complex flow reactors.
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